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Band discontinuities at heterojunctions between crystalline and amorphous silicon

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Heterojunctions between amorphous silicon (a-Si) and crystalline silicon (c-Si) can be used to improve the performance of solar cells and of heterojunction bipolar transistors. In addition, they enable the study of the amorphous-crystalline interface, and may provide more information about density of states and other electronic or structural properties of a-Si. One of the key properties of the heterojunction, namely the band lineup at the a-Si/c-Si interface, has been a subject of controversy. Experimental results range from zero offset in the valence band[1,2] to zero offset in the conduction band.[3,4] We have performed a theoretical investigation of this issue, based on first-principles calculations for the electronic structure of a-Si and c-Si, and the model-solid theory.[5]

The theoretical predictions highlight the fact that a major uncertainty arises because of the lack of information about the density of a-Si. Indeed, the density of the material affects the position of the average electrostatic potential, and hence the value of the band discontinuities. Recent experimental results indicate that a-Si is 1.8% less dense than c-Si.[6] Using this value, we find a valence-band offset close to zero. However, the offset may increase if the density of a-Si is higher in the near-interface region. The density of a-Si is affected by the presence of voids, which may make the material appear less dense on a macroscopic scale than it is on a microscopic scale. We will discuss experimental determinations of the density and of the band discontinuities, and also address the effect of hydrogen incorporation in the amorphous material.

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